Comput Stat (2013) 28:255–268
DOI 10.1007/s00180-011-0297-6

ORIGINAL PAPER

An efficient simulation algorithm for the generalized von Mises distribution of order two

Samuel Pfyffer · Riccardo Gatto

Received: 23 December 2009 / Accepted: 18 December 2011 / Published online: 31 December 2011

Abstract In this article we propose an exact efficient simulation algorithm for the generalized von Mises circular distribution of order two. It is an acceptance-rejection algorithm with a piecewise linear envelope based on the local extrema and the inflexion points of the generalized von Mises density of order two. We show that these points can be obtained from the roots of polynomials and degrees four and eight, which can be easily obtained by the methods of Ferrari and Weierstrass. A comparative study with the von Neumann acceptance-rejection, with the ratio-of-uniforms and with a Markov chain Monte Carlo algorithms shows that this new method is generally the most efficient.

Keywords Acceptance-rejection algorithm · Bimodality · Circular distribution · Markov chain Monte Carlo · Methods of Ferrari and Weierstrass · Piecewise linear envelope · Ratio-of-uniforms algorithm

Mathematics Subject Classification (2000) 65C10 · 62H11

Research partially supported by the Swiss National Science Foundation.

S. Pfyffer
Physics Institute, Space Research and Planetary Sciences, University of Bern,
Sidlerstrasse 5, 3012 Bern, Switzerland
e-mail: samuel.pfyffer@space.unibe.ch

R. Gatto (✉)
Institute of Mathematical Statistics and Actuarial Science, University of Bern,
Alpeneggstrasse 22, 3012 Bern, Switzerland
e-mail: gatto@stat.unibe.ch

1 Introduction

In this article we provide an efficient method for generating pseudo-random numbers from the generalized von Mises distribution of order two, which is a "circular" distribution with interesting practical and theoretical properties. Circular distributions are relevant in disciplines where observations take the form of two-dimensional directions. These observations can be represented as points on the unit circle or as angles and are referred to as circular data. Examples can be found in various domains. In geology, an analysis of paleocurrents to infer about the directions of flow of rivers in the past is presented in Sengupta and Rao (1967). In ornithology, an analysis of flight directions of birds is presented in Schmidt-Koenig (1963). In meteorology, the correlation between wind directions and ozone levels is studied in Johnson and Wehrli (1977). Circular data arise also from periodic phenomena with known periods, like circadian rhythms in medicine, daily occurrence of road accidents, etc. For an historical introduction with applications refer to Fisher (1993, Section 1). Two other recent monographs on circular statistics are Jammalamadaka and SenGupta (2001) and Mardia and Jupp (2000). A circular density is a non-negative 2π-periodic function defined on $\mathbb{R}$ integrating to one on $[0, 2\pi)$ and therefore on any shift of it. A class of circular densities with interesting theoretical and practical properties is given by

$$f(\theta \mid \mu_1, \ldots, \mu_k, \kappa_1, \ldots, \kappa_k) = \frac{1}{2\pi G_0^{(k)}(\delta_1, \ldots, \delta_{k-1}, \kappa_1, \ldots, \kappa_k)} \exp\left\{\sum_{j=1}^{k} \kappa_j \cos j(\theta - \mu_j)\right\}, \quad (1)$$

for $\theta \in \mathbb{R}$, where $\kappa_j \geq 0$, $\mu_j \in [0, 2\pi/j)$, for $j = 1, \ldots, k$,

$$G_0^{(k)}(\delta_1, \ldots, \delta_{k-1}, \kappa_1, \ldots, \kappa_k) = \frac{1}{2\pi} \int_0^{2\pi} \exp\{\kappa_1 \cos\theta + \kappa_2 \cos 2(\theta + \delta_1) + \cdots + \kappa_k \cos k(\theta + \delta_{k-1})\} d\theta, \quad (2)$$

and where $\delta_1 = (\mu_1 - \mu_2) \bmod \pi$, $\delta_2 = (\mu_1 - \mu_3) \bmod (2\pi/3)$, $\ldots$, $\delta_{k-1} = (\mu_1 - \mu_k) \bmod (2\pi/k)$. Gatto and Jammalamadaka (2007) called (1) the "generalized von Mises of order k" (GvM_k) density and denoted a circular random variable θ with this density by $\theta \sim \mathsf{GvM}_k(\mu_1, \ldots, \mu_k, \kappa_1, \ldots, \kappa_k)$. Some results of computational nature related to GvM_2 distributions are given in Gatto (2008), some information theoretic results related to GvM_k distributions are given in Gatto (2009) and relationships between GvM_k distributions and "generalized von Mises–Fisher" distributions on the unitary hypersphere are given in Gatto (2010). The GvM_1 distribution is the well-known circular normal or von Mises (vM) distribution, given by $f(\theta \mid \mu, \kappa) = \{2\pi I_0(\kappa)\}^{-1} \exp\{\kappa \cos(\theta - \mu)\}$, for $\theta \in \mathbb{R}, \mu \in [0, 2\pi), \kappa > 0$, where $I_n(z) = (2\pi)^{-1} \int_0^{2\pi} \cos n\theta \exp\{z \cos\theta\} d\theta$, $z \in \mathbb{C}$, is the modified Bessel function of the first kind and integer order n (see e.g. Abramowitz and Stegun 1972, p. 376). In this article we focus on the GvM_2 distribution, which will be simply called GvM

and we will denote $\mathsf{GvM}(\mu_1, \mu_2, \kappa_1, \kappa_2) = \mathsf{GvM}_2(\mu_1, \mu_2, \kappa_1, \kappa_2)$. Compared to the vM, which is only circular symmetric and unimodal, the GvM distribution allows for substantially higher flexibility in terms of asymmetry and bimodality. Also, GvM distributions offer various advantages with respect to mixtures of two vM distributions, for example, which are listed in Gatto (2008, p. 322 and 323).

There are some particular difficulties in constructing simple algorithms for generation of random variables from the GvM distribution. These difficulties arise essentially from the following facts. First, the complexity of the normalizing constant (2) excludes the construction of algorithms based on simple methods like the inverse transform or the composition methods. This constant could be evaluated by the Fourier expansion (3) below, but this would be inefficient in the context of simulation. Second, the non-availability of a numerically efficient formula for the inverse of the GvM distribution function. The GvM distribution function is available as infinite sum only, see Gatto (2008, Equation 25). Third, the non-existence of invariance properties which would allow to focus the analysis on a standardized version of the GvM distribution. If it would be possible to express any GvM random variable as a transform of a standardized one, i.e. from one with μ_1, μ_2, κ_1 and κ_2 fixed to some standard values, then it would be substantially easier to develop specific simulation algorithms for that particular standard GvM random variable only. For example, normal random variables are generated by linear transformations of standard normal random variables, which can be generated by the Box–Müller algorithm. Fourth and last, the bimodality of the density prevents direct applications of algorithms requiring log-concavity or log-convexity of the density, as proposed e.g. by Gilks (1992), Gilks and Wild (1992) and Gilks et al. (1995). General algorithms requiring concavity or convexity of the density can however be applied locally, after considering an appropriate partition of the domain of the density, see for example Evans and Swartz (1998). The generation algorithm that we propose for the GvM distribution does also exploit the local concavity and convexity of the density. It is an acceptance-rejection algorithm with a piecewise linear envelope obtained from the local extrema (i.e. the stationary points) and the inflexion points of the GvM density. We show that all these local extrema and inflexion points can be obtained by searching the roots of polynomials of degrees four and eight. For the quartic equation we apply the method of Ferrari, which dates back to Tartaglia, Cardan and Ferrari in the 1540's and which provides exact solutions; see e.g. Borofsky (1950, Section 8.7). Note that an alternative determination of the exact roots of the quartic equation is given by Beji (2008). For the degree eight we can apply the method of Weierstrass, also called method of Durand–Kerner, which was introduced by Weierstrass in 1891, further analyzed by Durand (1960) and which finds iteratively the roots of polynomials of any degree; see e.g. Dahlquist and Björk (2008, Section 6.5.4) or the short summary in Gatto (2008, Section 3.2). We provide the formulae for the coefficients of these polynomials. A comparative study with the von Neumann acceptance-rejection (with constant envelope), with the ratio-of-uniforms and with a Markov chain Monte Carlo algorithms shows that this new method is generally the most efficient in the sense that it yields the lowest rejection rate. The ratio-of-uniforms algorithm is due to Kinderman and Monahan (1977) and the application to the GvM distribution can be found in Gatto (2008, Section 3). Note finally that a particular acceptance-rejection algorithm for the vM distribution is given by Best and Fisher (1978).

The remaining part of this article is organized as follows. The presentation of the new acceptance-rejection algorithm is given in Sect. 2. A comparative numerical study with the other algorithms just mentioned is given in Sect. 3. Some concluding remarks are given in Sect. 4. Some technical developments are given in the "Appendix".

2 The simulation algorithm

In this section we propose an efficient acceptance-rejection simulation algorithm for the bimodal $\mathsf{GvM}(\mu_1, \mu_2, \kappa_1, \kappa_2)$ random variable. Acceptance-rejection algorithms are amongst the most popular methods for generating random variables, see e.g. Ripley (1987, Section 3.2) or Rubinstein and Kroese (2008, Section 2.3.4). We first give a general form of the acceptance-rejection algorithm adapted to the GvM distribution. For simplicity, let us re-write $\delta = \delta_1(=(\mu_1 - \mu_2) \bmod \pi)$ and $G_0 = G_0^{(2)}$, which admits the Fourier expansion

$$G_0(\delta, \kappa_1, \kappa_2) = I_0(\kappa_1) I_0(\kappa_2) + 2 \sum_{j=1}^{\infty} I_{2j}(\kappa_1) I_j(\kappa_2) \cos 2j\delta. \tag{3}$$

General form of the acceptance-rejection algorithm for the GvM distribution

Step 1. Find a decomposition

$$f(\theta|\mu_1, \mu_2, \kappa_1, \kappa_2) = \frac{c}{G_0(\delta, \kappa_1, \kappa_2)} \cdot d(\theta) \cdot s(\theta),$$

for $\theta \in \mathbb{R}$, where $c \in [G_0(\delta, \kappa_1, \kappa_2), \infty)$ is a constant, $d : \mathbb{R} \to (0, \infty)$ is a circular density and $s : \mathbb{R} \to (0, 1]$ is a 2π-periodic function.

Step 2. Generate U from the uniform distribution on $[0, 1)$ and $\tilde{\theta}$ from the density $d(\theta)$, for $\theta \in [0, 2\pi)$.

Step 3. If $U \leq s(\tilde{\theta})$, then consider $\theta = \tilde{\theta}$ as a $\mathsf{GvM}(\mu_1, \mu_2, \kappa_1, \kappa_2)$ pseudo-random number and stop. Else, reject both U and $\tilde{\theta}$ and go to Step 2. Iterate steps 2 and 3.

So far, the above algorithm is only conceptual, as it does not provide details on the decomposition in Step 1. The product $h = c/G_0(\delta, \kappa_1, \kappa_2) \cdot d$ is called envelope and s is a shrinkage function, in the sense that it shrinks the envelope h against $f = f(\cdot|\mu_1, \mu_2, \kappa_1, \kappa_2)$ by multiplication by s. There are many ways of choosing the decomposition in Step 1 and it is convenient to choose the envelope as close as possible to f with the density d allowing for simple generation. We note that the decomposition of f in Step 1 does not require evaluating the constant $G_0(\delta, \kappa_1, \kappa_2)$ (because this constant disappears after multiplying both sides of the equation by it) and, more important, the evaluation of $G_0(\delta, \kappa_1, \kappa_2)$ is neither required in the iterations of Steps 2 and 3 above. The ratio number of acceptances over number of iterations is called efficiency and it is here given by $\varepsilon = c^{-1}$. Also, the number of trials for a successful generation is a geometric random variable with expectation $c/G_0(\delta, \kappa_1, \kappa_2) \in [1, \infty)$. The von

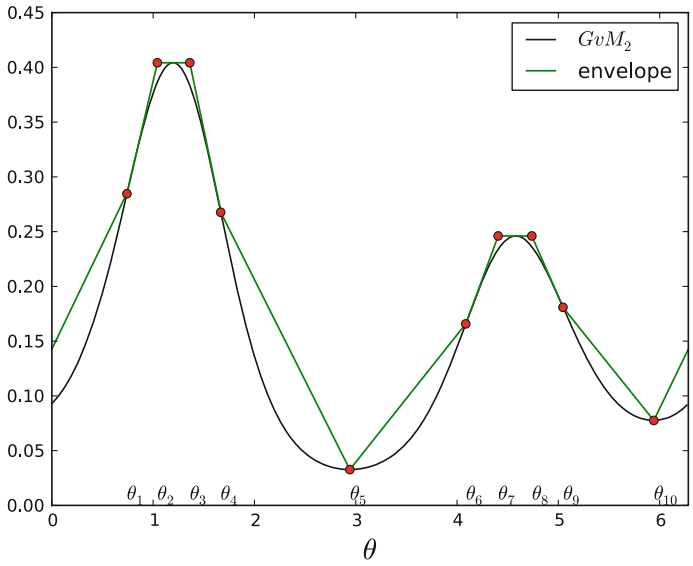

Fig. 1 The GvM$(15°, 75°, 0.5, 0.9)$ density with the corresponding piecewise linear envelope

Neumann algorithm is the acceptance-rejection algorithm with constant envelope h and the best constant envelope is clearly $h(\theta) = \sup_{\omega\in[0,2\pi)} f(\omega|\mu_1, \mu_2, \kappa_1, \kappa_2), \forall\theta \in \mathbb{R}$. (This most efficient von Neumann algorithm for the GvM distribution is given in Gatto 2008, p. 327, with two misprints: g is actually e^g in both Steps $1''$ and $3''$). In the numerical comparisons of Sect. 3, we consider this most efficient von Neumann algorithm.

We now propose the following improved envelope h, which is based on tangents to the density over circular regions of concavity and on secants over circular regions of convexity. Consider the set of abscissae of all local extrema and inflexion points of the bimodal GvM density f over $[0, 2\pi)$. Without loss of generality, let us assume that the smallest element of this set is the abscissa of an inflexion point and that the second smallest element is on the immediate left of the abscissa of a local maximum. This situation can always be obtained after shifting the GvM density f horizontally and an example is shown in Fig. 1. In this situation, we can define $0 \leq \theta_1 < \cdots < \theta_{10} < 2\pi$ as follows: θ_5 and θ_{10} are the abscissae of the two local minima of f; $\theta_1, \theta_4, \theta_6$ and θ_9 are the abscissae of the four inflexion points of f; θ_2 and θ_3 are the abscissae of the two points of intersection between the tangent line at the local maximum of f and the tangent lines at the two inflexion points of f, this for the left peak of f; and θ_7 and θ_8 are defined in an analogue manner for the right peak of f. Let us define $f_0(\theta) = G_0(\delta, \kappa_1, \kappa_2) \cdot f(\theta|\mu_1, \mu_2, \kappa_1, \kappa_2), \forall\theta \in \mathbb{R}$. An envelope for f_0 is provided by the piecewise linear continuous function

$$h_0(\theta) = \begin{cases} a_1(\theta \bmod 2\pi), & \text{if } \theta \bmod 2\pi \in [0, \theta_1), \\ \vdots & \vdots \\ a_{11}(\theta \bmod 2\pi), & \text{if } \theta \bmod 2\pi \in [\theta_{10}, 2\pi), \end{cases} \tag{4}$$

where $\theta \in \mathbb{R}$, a_i denotes the affine function which joins the point $(\theta_{i-1},\ f_{0i-1}(\theta_{i-1}))$ to the point $(\theta_i,\ f_{0i}(\theta_i))$, $i = 1, \ldots, 11$, $\theta_0 \stackrel{\text{def}}{=} \theta_{10} - 2\pi$, $\theta_{11} \stackrel{\text{def}}{=} \theta_1 + 2\pi$, $f_{0i} = f_0$, for $i = 0, 1, 4, 5, 6, 9, 10, 11$, $f_{02} = f_{03}$ have the value of the left local maximum and $f_{07} = f_{08}$ have the value of the right local maximum. Clearly, $f_0(\theta) \leq h_0(\theta)$, $\forall \theta \in \mathbb{R}$. Hence $h = h_0/G_0$ is a piecewise linear envelope for f. Though, computing h_0 alone is sufficient for the acceptance-rejection algorithm. Figure 1 gives an illustration of the piecewise linear envelope $h(\theta)$ of $f(\theta|15°, 75°, 0.5, 0.9)$ for $\theta \in [0, 2\pi)$. A systematic way of obtaining the set of abscissae of all local extrema and inflexion points entails various detailed operations and it is therefore deferred to the "Appendix".

Based on these developments, we propose the following algorithm for generating a bimodal $\mathsf{GvM}(\mu_1, \mu_2, \kappa_1, \kappa_2)$ random variable on $[0, 2\pi)$.

Acceptance-rejection algorithm for the GvM distribution with piecewise linear envelope

Step 0. If necessary, shift the GvM density so that, starting from the left, the first of all local extrema or inflexion points over $[0, 2\pi)$ is an inflexion point and the second is a local maximum.

Step 1. Search for the roots of the polynomials of degrees 4 and 8, given by (10) and (13) in the "Appendix". This can be done with the methods of Ferrari for the degree four and with the method of Weierstrass for the degree eight. Transform these roots to angles by (11) and (12). Deduce the local extrema and the inflexion points by evaluating $f(\cdot|\mu_1, \mu_2, \kappa_1, \kappa_2)$ at these angles. Based on these points, construct the piecewise linear envelope h_0 to $f_0 = G_0(\delta, \kappa_1, \kappa_2) \cdot f$ as given in (4).

Step 2. Generate U from the uniform distribution on $[0, 1)$ and $\tilde{\theta}$ from the density $d(\theta) = h_0(\theta)/\int_0^{2\pi} h_0(\omega)d\omega$, for $\theta \in [0, 2\pi)$. The generation from d can be done by the composition method as follows: generate U' from the uniform distribution on $[0, 2\pi)$ and generate $\tilde{\theta}$ from the normalized affine function a_i over $[\theta_{i-1}, \theta_i)$, if $U' \in [\theta_{i-1}, \theta_i)$, $i = 2, \ldots, 10$, or from the normalized function affine a_1 over $[\theta_0, \theta_1)$, if $U' < \theta_1$ or $U' > \theta_{10}$, with reduction modulo 2π in this latter case.

Step 3. Let $s = f_0/h_0$. If $U \leq s(\tilde{\theta})$, then consider $\theta = \tilde{\theta}$ as a $\mathsf{GvM}(\mu_1, \mu_2, \kappa_1, \kappa_2)$ pseudo-random number and stop. Else, reject both U and $\tilde{\theta}$ and go to Step 2. Iterate Steps 2 and 3.

Intuitively, the proposed envelope h is optimal in the sense of yielding a good reproduction of the bimodal shape of the GvM density, while remaining piecewise linear with a small number of edges. The generation from the linear functions is elementary and the number of comparisons is small. As mentioned is Remark 1, more refined envelopes could be obtained, although they would imply a larger number of comparisons.

Remark 1 Obviously, the piecewise linear envelope can be arbitrarily refined over the circular intervals having two circularly consecutive inflexion points as boundaries and

which contain a local minimum. In the previous configuration, these are the interval (θ_4, θ_6), which contains the local minimum θ_5, and the circular interval (θ_9, θ_1) (with $\theta_1 < \theta_9 \in [0, 2\pi)$), which contains θ_{10} as minimum. Since the GvM density is convex over (θ_4, θ_6), any straight line crossing two points $\big(\theta', f(\theta')\big)$ and $\big(\theta'', f(\theta'')\big)$, with $\theta_4 < \theta' < \theta'' < \theta_6$, will not intersect graph of the density over (θ', θ''). From this fact, we can easily construct envelopes which are arbitrarily close the GvM density by extending the number of secants over (θ_4, θ_6). The same holds for (θ_9, θ_1). The analogue refinement can be considered over the intervals of concavity (θ_1, θ_4) and (θ_6, θ_9), by extending the number of tangents. This refinement of the envelope could be carried out adaptively. That is, if $\tilde{\theta}$ generated from Step 2 above is rejected and if either $\tilde{\theta} \in (\theta_4, \theta_6)$ or $\tilde{\theta} \in (\theta_9, \theta_1)$, circularly, then the point $(\tilde{\theta}, f(\tilde{\theta}))$ is considered as a new vertex of the updated envelope.

Remark 2 We can also construct a simple piecewise constant envelope which improves the best von Neumann algorithm. We first determine the two local maxima and minima in $[0, 2\pi)$ by searching the roots of the fourth degree polynomial (10). Then, over each one of the two circular intervals in $[0, 2\pi)$ having two circularly consecutive minima as boundaries, we determine the constant function which crosses the maximum over the interval. We finally sum these two constant functions and obtain the piecewise constant envelope. A more refined piecewise constant envelope could be constructed by using the inflexion points as well. But this envelope could not be better than the proposed piecewise linear envelope while its computational burden for simulation would be close to the one of the piecewise linear envelope.

Remark 3 For globally log-concave or log-convex densities, an envelope can be constructed from a set of tangents to the log-density, as suggested by Gilks and Wild (1992), or from a set of secants to the log-density, as suggested by Gilks (1992). This type of densities appear often in Bayesian models as full conditionals within Gibbs sampling. Even without the required log-concavity or log-convexity, these methods provide approximations to the density and they are used within the Metropolis algorithm, yielding high acceptance rates whenever the density is approximately log-concave or log-convex, see Gilks et al. (1995). Our algorithm can be seen as a particular simultaneous application of these methods, as it decomposes the domain $[0, 2\pi)$ into circular regions of convexity and concavity and joins an envelope based on tangents, over circular regions of concavity, with another envelope based on secants, over circular regions of convexity.

Remark 4 The above algorithm can be refined by using squeezing or pretesting, see e.g. Ripley (1987, pp. 67–71). It is quite easy to obtain a lower squeezing function which would allow to skip many evaluations of the non-normalized GvM density. In order to construct the piecewise linear envelope h_0, we need to compute the local maxima and minima as well as the inflexion points of the GvM density f over $[0, 2\pi)$. With the same set of points, we can obtain a lower piecewise linear envelope or squeezing function l_0 such that $l_0(\theta) \leq f_0(\theta), \forall \theta \in \mathbb{R}$. Let us redefine the horizontal coordinates of the inflexion points $\theta_1, \theta_4, \theta_6, \theta_9$ as $\eta_2, \eta_4, \eta_7, \eta_9$, respectively, let us define by $\eta_3 < \eta_8$ the horizontal coordinates of the maxima and let us define by $\eta_1 < \eta_5 < \eta_6 < \eta_{10}$ the horizontal coordinates the points of intersection between the

straight lines through the local minima and the tangent lines through the neighboring inflexion points. Based on these points we define $l_0(\theta)$ as

$$l_0(\theta) = \begin{cases} b_1(\theta \bmod 2\pi), & \text{if } \theta \in [0, \eta_1)\,, \\ \vdots & \vdots \\ b_{11}(\theta \bmod 2\pi), & \text{if } \theta \in [\eta_{10}, 2\pi)\,, \end{cases} \tag{5}$$

where $\theta \in \mathbb{R}$, b_i denotes the affine function which joins the point $(\eta_{i-1},\, f_{0i-1}(\eta_{i-1}))$ to the point $(\eta_i,\, f_{0i}(\eta_i))$, $i = 1, \ldots, 11$, $\eta_0 \stackrel{\text{def}}{=} \eta_{10} - 2\pi$, $\eta_{11} \stackrel{\text{def}}{=} \eta_1 + 2\pi$, $f_{0i} = f_0$, for $i = 2, 3, 4, 7, 8, 9, 10, 11$, $f_{00} = f_{01}$ have the value of the left local minimum and $f_{05} = f_{06}$ have the value of the right local minimum. Hence $l = h_0/G_0$ is a piecewise linear lower squeezing function for the GvM density f. Given both upper and lower envelopes h_0 and l_0, the squeezed version of the above algorithm is obtained by inserting Step 2′ given below between Steps 2 and 3 in the above algorithm.

Step 2′. If $U \leq l_0(\tilde{\theta})/h_0(\tilde{\theta})$, accept $\theta = \tilde{\theta}$ as a $\mathsf{GvM}(\mu_1, \mu_2, \kappa_1, \kappa_2)$ pseudo-random number and stop.

Note however that both the piecewise linear envelope h_0 and the non-normalized GvM density f_0 are fast to evaluate. Consequently, this squeezing algorithm is not expected to enhance the performance significantly.

3 Numerical comparisons with other methods

In this section we show some numerical comparisons between the acceptance-rejection method with the new piecewise linear envelope and three competing methods, which are: the most efficient von Neumann method, explained at the beginning of Sect. 2, the ratio-of-uniforms, given in Gatto (2008, Section 3) and a Markov chain Monte Carlo method.

Markov chain Monte Carlo is a method of iterative simulation and the central idea is to generate iteratively from the transition (or jumping) distributions of a Markov chain having the desired (or target) distribution as stationary distribution. From the fact that the transition distributions converge towards the stationary distribution, all generations obtained after discarding the first generations (or after a burn-in period) can be considered as generations from the stationary distribution. In the Metropolis algorithm, the jumping distribution can take a simple form, irrespectively of the complexity of the target distribution, which can have a complicated form. The method originated from statistical physics see Metropolis et al. (1953), see also Asmussen and Glynn (2007, Chapter 13) or Rubinstein and Kroese (2008, Chapter 6), for example. In our case we have the GvM target distribution and we select the uniform jumping distribution. Given that the GvM distribution is considered over a bounded domain and that it is generally not unimodal, the uniform jumping distribution is a sensible choice and it allows for the fastest generation. This leads to the following algorithm.

Table 1 Numerical comparisons between the von Neumann (vN), ratio-of-uniforms (RU), Markov chain (MC) and piecewise linear envelope (PL) simulation methods for $\mu_1 = 0$ and various combinations of δ, κ_1 and κ_2

Parameters	vN	RU	MC	PL
$\kappa_1, \kappa_2, \delta$	ε, n	ε, n	ε, n	ε, n
1.0, 1.0, 0°	0.2382, 251853	0.3149, 190567	0.4479, 133963	0.7580, 79160
0.1, 1.0, 60°	0.3732, 160766	0.6593, 91000	0.6148, 97588	0.8404, 71396
1.0, 1.0, 90°	0.4718, 127166	0.7782, 77104	0.6157, 97445	0.8468, 70852
1.5, 1.1, 117°	0.2734, 219470	0.3959, 151567	0.4839, 123985	0.7847, 76465
1.0, 2.0, 140°	0.1817, 330263	0.2011, 298436	0.3392, 176868	0.6538, 91773

ε: ratio of acceptances over number of iterations or efficiency. n: number of iterations in order to reach 60,000 acceptances. Markov chain burn-in iterations, not included in n: 2000. Starting point for Markov chain: 0.0852

Markov chain Monte Carlo algorithm for the GvM distribution with uniform jumping distribution

Step 1. Select any starting point $\theta_0 \in [0, 2\pi)$.
Step 2. Generate θ^* from the uniform jumping density on $[0, 2\pi)$. Set

$$r = \frac{f(\theta^*|\mu_1, \mu_2, \kappa_1, \kappa_2)}{f(\theta_0|\mu_1, \mu_2, \kappa_1, \kappa_2)} \quad \text{and} \quad p = \min\{r, 1\}.$$

Step 3. Generate U from the uniform distribution on $[0, 1)$ and set

$$\theta = \begin{cases} \theta^*, & \text{if } p \geq U, \\ \theta_0, & \text{if } p < U. \end{cases}$$

Iterate Steps 2 and 3 with $\theta_0 = \theta$.

Table 1 shows numerical comparisons of the acceptance-rejection method based on the piecewise linear envelope with its direct competitors, which are the von Neumann, the ratio-of-uniforms and a Markov chain algorithms. For $\mu_1 = 0$ and the values of δ, κ_1 and κ_2 given in the first column of Table 1, we see that the new method with the piecewise linear envelope is always the most efficient, in the sense of yielding the smallest number of rejections for the total number of iterations. The ratio-of-uniforms and Markov chain methods show comparable efficiencies here, which are however substantially lower than the efficiency of the proposed piecewise linear envelope. The von Neumann method systematically shows the lowest efficiencies and this could have been expected. However, the efficiencies of the von Neumann method are given in Table 1 mainly to illustrate the relative improvement of the three other methods with respect to a basic method. Note that there exist more refined choices of jumping distribution for Markov chain Monte Carlo, as e.g. the adaptive piecewise linear approximation of Gilks et al. (1995). These choices should lead to ratios of acceptances higher than under the uniform jumping distribution used here, however they would also increase

the overall complexity and hence the computing time of the Metropolis algorithm. A good jumping distribution should allow for simple sampling, for reasonably large jumps in the support of the target distribution (in order to obtain good mixing in the Markov chain) and should not reject the jumps too frequently. The uniform jumping distribution fulfills these three important criteria. Finally, we give the efficiencies of our piecewise linear envelope by direct evaluation of the area under the envelope and by numerical integration of the normalizing constant of the GvM density. For $\mu_1 = 0$ and the values of δ, κ_1 and κ_2 given in the first column of Table 1, going from first to last row, we obtain $\varepsilon = 0.7587, 0.8477, 0.8440, 0.7838, 0.6525$, respectively. These values are very close to the corresponding values given in the column PL of Table 1. The numerical results presented are based on the pseudo-random number generator of *Fortran 90*. The programs used for these computations are written in *Fortran 90* and the programs for the generation with the proposed piecewise linear envelope are available under http://www.stat.unibe.ch, after selecting *Research/Publications/Software*.

4 Conclusion

In this article we present an acceptance-rejection simulation algorithm for the GvM distribution, based on a tight piecewise linear envelope, and a numerical comparison with three alternative simulation methods. The numerical results lead to the following conclusions. For GvM densities with two modes of similar height, which can be obtained by setting $\kappa_1 \simeq \kappa_2$ and $\delta \simeq \pi/2$, the ratio-of-uniforms method appears quite close to the proposed method, based on the piecewise linear envelope. In general, for bimodal GvM densities, the best von Neumann simulation method produces high rejection rates, but it is the simplest method to implement. There are no clear advantages in using Markov chain Monte Carlo simulation: it requires discarding the first generations to ensure that the Markov chain has reached its stationary distribution, i.e. a burn-in period, and it does not lead to the same type of efficiencies as with the proposed piecewise linear envelope. Some ideas presented here could be extended for computing tight envelopes to other GvM_k densities with $k > 2$.

Acknowledgments The authors thank the Editor, the Co-Editor, the Associate Editor and two anonymous Reviewers for thoughtful suggestions and corrections which improved the quality of this article.

Appendix: The local extrema and the inflexion points of the generalized von Mises density

In this "Appendix" we show how to obtain the local extrema and inflexion points of $f(\theta|\mu_1, \mu_2, \kappa_1, \kappa_2)$, for $\theta \in [0, 2\pi)$. Some parts of this paragraph are from Gatto (2008, Section 3.2). Let us consider for the moment the density at points $\omega = \theta - \mu_1$ over $[0, 2\pi)$, where θ denotes the original abscissa. As $\delta = (\mu_1 - \mu_2) \bmod \pi$, the exponent of the GvM density expressed in terms of ω becomes

$$g(\omega) = \kappa_1 \cos \omega + \kappa_2 \cos 2(\omega + \delta).$$

The extrema are necessarily given by the roots of $d\, f(\omega|0, \delta, \kappa_1, \kappa_2)/d\omega$ and the inflexion points are necessarily given by the roots of $d^2 f(\omega|0, \delta, \kappa_1, \kappa_2)/d\omega^2$. We have

$$\frac{d}{d\omega} f(\omega|0, \delta, \kappa_1, \kappa_2) = \frac{d}{d\omega} g(\omega)\, f(\omega|0, \delta, \kappa_1, \kappa_2)$$

and

$$\frac{d^2}{d\omega^2} f(\omega|0, \delta, \kappa_1, \kappa_2) = \left(\frac{d^2}{d\omega^2} g(\omega) + \left(\frac{d}{d\omega} g(\omega) \right)^2 \right) f(\omega|0, \delta, \kappa_1, \kappa_2).$$

Since $f(\cdot|0, \delta, \kappa_1, \kappa_2)$ is positive, the search for these roots corresponds to solving

$$\frac{d}{d\omega} g(\omega) = 0$$

and

$$\frac{d^2}{d\omega^2} g(\omega) + \left(\frac{d}{d\omega} g(\omega) \right)^2 = 0, \tag{6}$$

respectively, which simplify to

$$-\kappa_1 \sin \omega \; - \; 2\kappa_2 \sin 2\,(\omega + \delta) = 0 \tag{7}$$

and to

$$-\kappa_1 \cos \omega - 4\kappa_2 \cos 2\,(\omega + \delta) + \{\kappa_1 \sin \omega + 2\kappa_2 \sin 2\,(\omega + \delta)\}^2 = 0, \tag{8}$$

respectively.

Concerning the local extrema, by expanding the sine and cosine functions, (7) can be rewritten as

$$(1 - 2\sin^2 \delta) \sin \omega \cos \omega - 2 \sin \delta \cos \delta \sin^2 \omega + \rho \sin \omega + \sin \delta \cos \delta = 0, \tag{9}$$

where $\rho = \kappa_1/(4\kappa_2)$. The bimodality of $f(\omega|0, \delta, \kappa_1, \kappa_2)$ is determined by the number of roots in $\omega \in [0, 2\pi)$ of (9). The substitution $x = \sin \omega$ in (9) yields

$$\pm \left(1 - 2\, \sin^2 \delta\right) x \sqrt{1 - x^2} = 2\, \sin \delta \cos \delta x^2 - \rho x - \sin \delta \cos \delta.$$

Taking the square on both sides of the above equation leads to searching for the roots in $x \in [-1, 1]$ of the polynomial

$$b_0 + b_1 x + b_2 x^2 + b_3 x^3 + x^4, \tag{10}$$

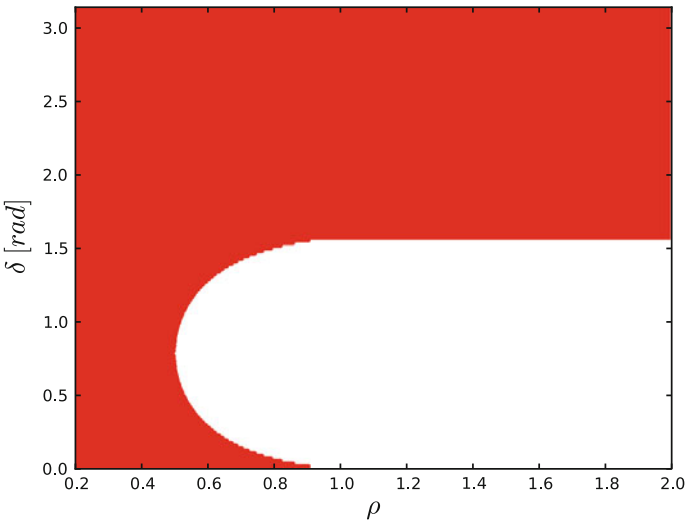

Fig. 2 Decomposition of the space of (ρ, δ) into the region giving bimodality, *shaded*, and the region giving unimodality, *empty*, of the GvM density

where the coefficients are given by

$$b_0 = \sin^2\delta\cos^2\delta,\ \ b_1 = 2\rho\sin\delta\cos\delta,\ \ b_2 = \rho^2 - 1\ \text{ and }\ b_3 = -4\rho\sin\delta\cos\delta.$$

As mentioned in Sect. 1, the roots of polynomial (10) can be determined exactly by the method of Ferrari. Next, we transform the roots of (10) back to the angular scale by

$$\omega = (\arcsin x) \bmod 2\pi,\ \ (\pi - \arcsin \mathrm{x}) \bmod 2\pi, \tag{11}$$

(with $\arcsin : [-1, 1] \to [-\pi/2, \pi/2]$) and finally to the original abscissa

$$\theta = (\omega + \mu_1) \bmod 2\pi. \tag{12}$$

The nature of the resulting extrema is then determined by the evaluation of $f(\cdot|\mu_1, \mu_2, \kappa_1, \kappa_2)$ at these points. In some cases, the fourth degree polynomial (10) can have two real roots only instead of four, which means that $f(\cdot|\mu_1, \mu_2, \kappa_1, \kappa_2)$ is unimodal instead of bimodal. For example, if $\delta = \pi/2$, then $b_0 = b_1 = b_3 = 0$ and the fourth degree polynomial has exactly two real roots, provided that $\rho > 1$. Although the number of roots of the quartic (10) is a function of δ and ρ only, this function seems difficult to determine analytically. Figure 2, which is obtained numerically, shows the partition of the domain of δ and ρ into regions leading to exactly two and four roots. These two regions are respectively regions of unimodality and bimodality of the GvM density. The region with four roots is shaded and the region with two roots only is empty, or white.

The procedure for obtaining the inflexion points is similar to the one for obtaining the extrema. We mainly apply similar substitutions and expansions to (8), instead of (7), and finally obtain a polynomial of degree eight, instead of four. The four inflexion points are among the roots in $x \in [-1, 1]$ of this polynomial, which is

$$c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4 + c_5 x^5 + c_6 x^6 + c_7 x^7 + c_8 x^8, \tag{13}$$

with coefficients given by

$$\begin{aligned}
c_0 &= -(256\kappa_2^3 + 512\kappa_2^4)\sin^6\delta - (64\kappa_2^2 + 128\kappa_2^3)\sin^2\delta - \kappa_1^2 + 16\kappa_2^2 + 256\kappa_2^4 \sin^8\delta \\
&\quad + (64\kappa_2^2 + 256\kappa_2^4 + 384\kappa_2^3)\sin^4\delta, \\
c_1 &= 256\kappa_1\kappa_2^3 \sin^3\delta\cos\delta + 32\kappa_1\kappa_2 \sin\delta\cos\delta - 256\kappa_1\kappa_2^3 \sin^5\delta\cos\delta, \\
c_2 &= 8\kappa_1^2\kappa_2 + \kappa_1^2 - 64\kappa_2^2 - 128\kappa_2^3 + 512\kappa_2^3 \sin^6\delta + (512\kappa_2^4 - 96\kappa_1^2\kappa_2^2 - 768\kappa_2^3)\sin^4\delta \\
&\quad + (-512\kappa_2^4 + 512\kappa_2^3 + 96\kappa_1^2\kappa_2^2 - 16\kappa_1^2\kappa_2)\sin^2\delta, \\
c_3 &= (16\kappa_1^3\kappa_2 - 32\kappa_1\kappa_2 - 192\kappa_1\kappa_2^2 - 256\kappa_1\kappa_2^3)\sin\delta\cos\delta + 512\kappa_1\kappa_2^3 \sin^5\delta\cos\delta \\
&\quad + (384\kappa_1\kappa_2^2 - 512\kappa_1\kappa_2^3)\sin^3\delta\cos\delta, \\
c_4 &= -32\kappa_1^2\kappa_2^2 + 64\kappa_2^2 + 384\kappa_2^3 + 256\kappa_2^4 + \kappa_1^4 + (512\kappa_2^4 - 768\kappa_2^3 - 256\kappa_1^2\kappa_2^2)\sin^2\delta, \\
&\quad + (256\kappa_1^2\kappa_2^2 - 512\kappa_2^4)\sin^4\delta, \\
c_5 &= (128\kappa_1\kappa_2^2 - 32\kappa_1^3\kappa_2 + 768\kappa_1\kappa_2^3)\sin\delta\cos\delta - 256\kappa_1\kappa_2^2 \sin^3\delta\cos\delta, \\
c_6 &= 32\kappa_1^2\kappa_2^2 - 256\kappa_2^3 - 512\kappa_2^4 - 256\kappa_1^2\kappa_2^2 \sin^4\delta + (512\kappa_2^3 + 256\kappa_1^2\kappa_2^2)\sin^2\delta, \\
c_7 &= -512\kappa_1\kappa_2^3 \sin\delta\cos\delta \quad \text{and} \\
c_8 &= 256\kappa_2^4.
\end{aligned}$$

These expressions arise from simple but lengthy algebraic manipulations. As mentioned in Sect. 1, the roots of polynomial (13) can be obtained iteratively by the method of Weierstrass. We transform the roots of (13) back to the angular scale by (11) and (12). We evaluate $f(\cdot|\mu_1, \mu_2, \kappa_1, \kappa_2)$ at these points and retain the inflexion points.

References

Abramowitz M, Stegun IE (1972) Handbook of mathematical functions with formulas, graphs, and mathematical tables, Dover, 9th Printing, New York; originally published by the National Bureau of Standards, USA, 10th Printing

Asmussen S, Glynn PW (2007) Stochastic simulation: algorithms and analysis. Springer, New York

Beji S (2008) A systematic approach to the exact roots of polynomials. Mediterr J Math 5:163–172

Best DJ, Fisher NI (1978) Efficient simulation of the von Mises distribution. Appl Stat 28:152–157

Borofsky S (1950) Elementary theory of equations. MacMillan, New York

Dahlquist G, Björk A (2008) Numerical methods in scientific computing, vol I. SIAM, Philadelphia

Durand E (1960) Solutions numériques des équations algébriques. Équations du Type $F(x) = 0$; Racines d'un Polynôme, Tome I, Masson, Paris

Evans M, Swartz TB (1998) Random variable generation using concavity properties of transformed densities. J Comput Graph Stat 7:514–528

Fisher NI (1993) Statistical analysis of circular data. Cambridge University Press, Cambridge

Gatto R (2008) Some computational aspects of the generalized von Mises distribution. Stat Comput 18:321–331
Gatto R (2009) Information theoretic results for circular distributions. Statistics 43:409–421
Gatto R (2010) The generalized von Mises-Fisher distribution. In: Wells MT, SenGupta A (eds) Advances in directional and linear statistics, A Festschrift for Sreenivasa Rao Jammalamadaka. Physica-Verlag, Berlin, pp 51–68
Gatto R, Jammalamadaka SR (2007) The generalized von Mises distribution. Stat Methodol 4:341–353
Gilks WR (1992) Derivative-free adaptive rejection sampling for Gibbs sampling. In: Bernardo J, Berger J, Dawid AP, Smith AFM (eds) Bayesian statistics, 4th edn. Oxford University Press, Oxford
Gilks WR, Best NG, Tan KKC (1995) Adaptive rejection Metropolis sampling. Appl Stat 44:455–472
Gilks WR, Wild P (1992) Adaptive rejection sampling for Gibbs sampling. Appl Stat 41:337–348
Jammalamadaka SR, SenGupta A (2001) Topics in circular statistics. World Scientific Press, Singapore
Johnson RA, Wehrli TE (1977) Measures and models for angular correlation and angular-linear correlation. J R Stat Soc 39:222–229
Kinderman AJ, Monahan JF (1977) Computer generation of random variables using the ratio of uniform deviates. ACM Trans Math Softw 3:257–260
Mardia KV, Jupp PE (2000) Directional statistics. Wiley, Chichester
Metropolis N, Rosenbluth AW, Rosenbluth MN, Teller AH, Teller E (1953) Equation of state calculations by fast computing machines. J Chem Phys 21:1087–1092
Ripley BD (1987) Stochastic simulation. Wiley, New York
Rubinstein RY, Kroese DP (2008) Simulation and the Monte Carlo method, 2nd edn. Wiley, New Jersey
Schmidt-Koenig K (1963) On the role of loft, the distance and site of release in pigeon homing (the "cross-loft experiment"). Biol Bull 125:154–164
Sengupta S, Rao JS (1967) Statistical analysis of crossbedding azimuths from the Kamthi formation around Bheemaram, Pranhita Godavari valley. Sankhyā 28:165–174